(1,1'-Biphenyl)-2,2'-diol 1806-29-7 | DTXSID6051809

Model Performance

Model	Data	

Weighted KNN model

5-fold CV (75%)		Training (75	Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.89	0.25	0.88	0.26	0.75	0.38	

Model Results

Predicted value: 24.2 days

Global applicability domain: Outside

Local applicability domain index: 3.09e-01

Confidence level: 7.66e-01

Nearest Neighbors from the Training Set

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9-Ethyl-9H-fluorene Measured: 2330 Predicted: N/A

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2-Methylphenanthrene Measured: 1370 Predicted: 25.0

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4-Phenyltoluene Measured: 4340 Predicted: 25.1

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2-Methylnaphthalene Measured: 436 Predicted: 15.3

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1-Methyl phenanthrene Measured: 1370 Predicted: 36.9